High-Precision Arithmetic and Experimental Mathematics

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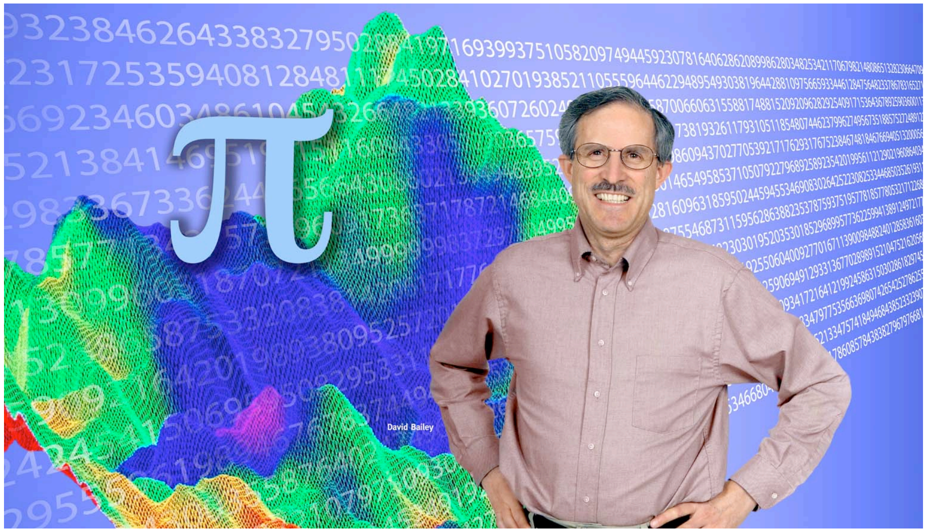


Applications of High-Precision Arithmetic in Modern Scientific Computing

- Highly nonlinear computations.
- Computations involving highly ill-conditioned linear systems.
- Computations involving data with very large dynamic range.
- Large computations on highly parallel computer systems.
- Computations where numerical sensitivity is not currently a major problem, but periodic testing is needed to ensure that results are reliable.
- Research problems in mathematics and mathematical physics that involve constant recognition and integer relation detection.

Few physicists, chemists or engineers are highly expert in numerical analysis. Thus high-precision arithmetic is often a better remedy for severe numerical round-off error, even if the error could, in principle, be improved with more advanced algorithms or coding techniques.

LBNL's High-Precision Software

- QD: double-double (31 digits) and quad-double (62 digits).
- ARPREC: arbitrary precision.
- Low-level routines written in C++.
- C++ and Fortran-90 translation modules permit use with existing C++ and Fortran-90 programs -- only minor code changes are required.
- Includes many common functions: sqrt, cos, exp, gamma, etc.
- PSLQ, root finding, numerical integration.

Available at: **http://www.experimentalmath.info**

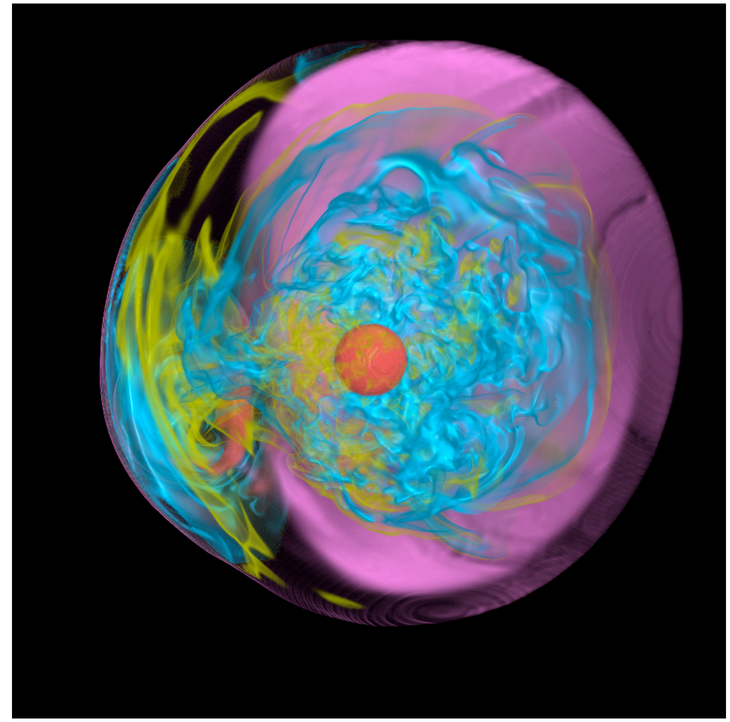
Authors: Xiaoye Li, Yozo Hida, Brandon Thompson and DHB

Some Real-World Applications of High-Precision Arithmetic

- Supernova simulations (32 or 64 digits).
- Climate modeling (32 digits).
- Planetary orbit calculations (32 digits).
- Coulomb n-body atomic system simulations (32-120 digits).
- Schrodinger solutions for lithium and helium atoms (32 digits).
- Electromagnetic scattering theory (32-100 digits).
- Studies of the fine structure constant of physics (32 digits).
- Scattering amplitudes of quarks, gluons and bosons (32 digits).
- Theory of nonlinear oscillators (64 digits).

Application of High-Precision Arithmetic: Supernova Simulations

- Researchers at LBNL are using QD to solve for non-local thermodynamic equilibrium populations of iron and other atoms in the atmospheres of supernovas.
- Iron may exist in several species, so it is necessary to solve for all species simultaneously.
- Since the relative population of any state from the dominant state is proportional to the exponential of the ionization energy, the dynamic range of these values can be very large.
- The quad-double portion now dominates the entire computation.



P. H. Hauschildt and E. Baron, “The Numerical Solution of the Expanding Stellar Atmosphere Problem,” *Journal Computational and Applied Mathematics*, vol. 109 (1999), pg. 41-63.

Coulomb N-Body Atomic System Simulations

- Alexei Frolov of Queen's University in Canada has used MPFUN90 to solve a generalized eigenvalue problem that arises in Coulomb n-body interactions.
- Matrices are typically 5,000 x 5,000 and are very nearly singular.
- Frolov has also computed elements of the Hamiltonian matrix and the overlap matrix in four- and five-body systems.
- These computations typically require 120-digit arithmetic.

"We can consider and solve the bound state few-body problems which have been beyond our imagination even four years ago." – Frolov

A. M. Frolov and DHB, "Highly Accurate Evaluation of the Few-Body Auxiliary Functions and Four-Body Integrals," *Journal of Physics B*, vol. 36, no. 9 (14 May 2003), pg. 1857-1867.

The PSLQ Integer Relation Algorithm

Let (x_n) be a given vector of real numbers. An integer relation algorithm finds integers (a_n) such that

$$a_1 x_1 + a_2 x_2 + \cdots + a_n x_n = 0$$

(or within "epsilon" of zero, where epsilon = 10^{-p} and p is the precision).

At the present time the "PSLQ" algorithm of mathematician-sculptor Helaman Ferguson is the most widely used integer relation algorithm. It was named one of ten "algorithms of the century" by *Computing in Science and Engineering*.

PSLQ (or any other integer relation scheme) requires very high precision (at least $n*d$ digits, where d is the size in digits of the largest a_k), both in the input data and in the operation of the algorithm.

1. H. R. P. Ferguson, DHB and S. Arno, "Analysis of PSLQ, An Integer Relation Finding Algorithm," *Mathematics of Computation*, vol. 68, no. 225 (Jan 1999), pg. 351-369.
2. DHB and D. J. Broadhurst, "Parallel Integer Relation Detection: Techniques and Applications," *Mathematics of Computation*, vol. 70, no. 236 (Oct 2000), pg. 1719-1736.

The BBP Formula for Pi

In 1996, at the suggestion of Peter Borwein, Simon Plouffe used DHB's PSLQ program and arbitrary precision software to discover this new formula for pi:

$$\pi = \sum_{n=0}^{\infty} \frac{1}{16^k} \left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right)$$

This formula permits one to compute binary (or hexadecimal) digits of pi beginning at an arbitrary starting position, using a very simple scheme that can run on any system with standard 64-bit or 128-bit arithmetic.

Recently it was proven that no base-n formulas of this type exist for pi, except $n = 2^m$.

1. DHB, P. B. Borwein and S. Plouffe, "On the Rapid Computation of Various Polylogarithmic Constants," *Mathematics of Computation*, vol. 66, no. 218 (Apr 1997), pg. 903-913.
2. J. M. Borwein, W. F. Galway and D. Borwein, "Finding and Excluding b-ary Machin-Type BBP Formulae," *Canadian Journal of Mathematics*, vol. 56 (2004), pg 1339-1342.

Tanh-Sinh Quadrature

Given $f(x)$ defined on (-1,1), define $g(t) = \tanh(\pi/2 \sinh t)$. Then setting $x = g(t)$ yields

$$\int_{-1}^{1} f(x)\, dx \;=\; \int_{-\infty}^{\infty} f(g(t))g'(t)\, dt \;\approx\; h \sum_{j=-N}^{N} w_j f(x_j),$$

where $x_j = g(hj)$ and $w_j = g'(hj)$. Since $g'(t)$ goes to zero very rapidly for large t, the product $f(g(t))\, g'(t)$ typically is a nice bell-shaped function for which the Euler-Maclaurin formula implies that the simple summation above is remarkably accurate. Reducing h by half typically doubles the number of correct digits.

Tanh-sinh quadrature is the best integration scheme for functions with vertical derivatives or blow-up singularities at endpoints, or for any function at very high precision (> 1000 digits).

1. DHB, Xiaoye S. Li and Karthik Jeyabalan, “A Comparison of Three High-Precision Quadrature Schemes,” *Experimental Mathematics*, vol. 14 (2005), no. 3, pg. 317-329.
2. H. Takahasi and M. Mori, “Double Exponential Formulas for Numerical Integration,” Publications of RIMS, Kyoto University, vol. 9 (1974), pg. 721–741.

A Log-Tan Integral Identity

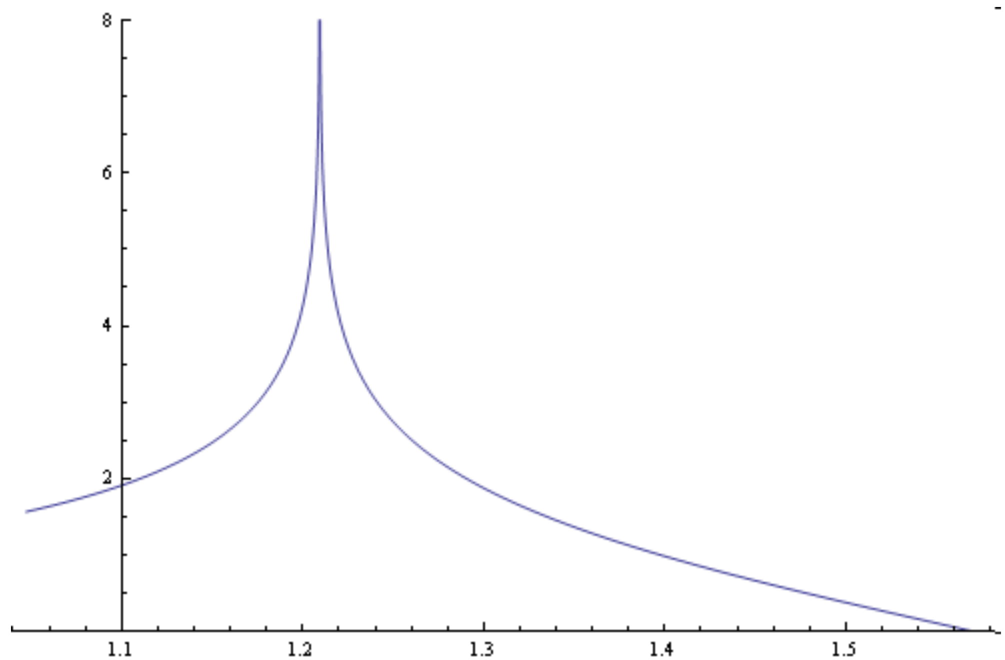
$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| \mathrm{d}t \quad = \quad L_{-7}(2) \quad =$$

$$\sum_{n=0}^{\infty} \left[\frac{1}{(7n+1)^2} + \frac{1}{(7n+2)^2} - \frac{1}{(7n+3)^2} + \frac{1}{(7n+4)^2} - \frac{1}{(7n+5)^2} - \frac{1}{(7n+6)^2} \right]$$

This identity arises from analysis of volumes of knot complements in hyperbolic space. This is simplest of 998 related identities.

We have verified this numerically to 20,000 digits (using highly parallel tanh-sinh quadrature). It has now been proven.

DHB, J. M. Borwein, V. Kapoor and E. Weisstein, "Ten Problems in Experimental Mathematics," *American Mathematical Monthly*, vol. 113, no. 6 (Jun 2006), pg. 481-409 .



Ising Integrals

We recently applied our methods to study three classes of integrals that arise in the Ising theory of mathematical physics – D_n and two others:

$$C_n := \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

$$D_n := \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{\prod_{i<j}\left(\frac{u_i-u_j}{u_i+u_j}\right)^2}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

$$E_n = 2\int_0^1 \cdots \int_0^1 \left(\prod_{1\le j<k\le n} \frac{u_k - u_j}{u_k + u_j}\right)^2 dt_2\, dt_3 \cdots dt_n$$

where in the last line $u_k = t_1\ t_2 \ldots t_k$.

DHB, J. M. Borwein and R. E. Crandall, "Integrals of the Ising Class," *Journal of Physics A: Mathematical and General*, vol. 39 (2006), pg. 12271-12302.

Computing and Evaluating C_n

We observed that the multi-dimensional C_n integrals can be transformed to 1-D integrals:

$$C_n = \frac{2^n}{n!} \int_0^\infty t K_0^n(t)\,\mathrm{d}t$$

where K_0 is the modified Bessel function. In this form, the C_n constants appear naturally in in quantum field theory (QFT).

We used this formula to compute 1000-digit numerical values of various C_n, from which the following results and others were found, then proven:

$$\begin{aligned}
C_1 &= 2 \\
C_2 &= 1 \\
C_3 &= \mathrm{L}_{-3}(2) = \sum_{n \geq 0} \left(\frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2} \right) \\
C_4 &= \frac{7}{12} \zeta(3)
\end{aligned}$$

Limiting Value of C_n

The C_n numerical values appear to approach a limit. For instance,

$$C_{1024} = 0.63047350337438679612204019271087890435458707871273234\ldots$$

What is this limit? We copied the first 50 digits of this numerical value into the online Inverse Symbolic Calculator (ISC):
http://ddrive.cs.dal.ca/~isc

The result was:

$$\lim_{n \to \infty} C_n = 2e^{-2\gamma}$$

where gamma denotes Euler's constant. Finding this limit led us to the asymptotic expansion and made it clear that the integral representation of C_n is fundamental.

Other Ising Integral Evaluations

$$
\begin{aligned}
D_2 &= 1/3 \\
D_3 &= 8 + 4\pi^2/3 - 27\,\mathrm{L}_{-3}(2) \\
D_4 &= 4\pi^2/9 - 1/6 - 7\zeta(3)/2 \\
E_2 &= 6 - 8\log 2 \\
E_3 &= 10 - 2\pi^2 - 8\log 2 + 32\log^2 2 \\
E_4 &= 22 - 82\zeta(3) - 24\log 2 + 176\log^2 2 - 256(\log^3 2)/3 \\
&\quad +16\pi^2\log 2 - 22\pi^2/3 \\
E_5 &\stackrel{?}{=} 42 - 1984\,\mathrm{Li}_4(1/2) + 189\pi^4/10 - 74\zeta(3) - 1272\zeta(3)\log 2 \\
&\quad +40\pi^2\log^2 2 - 62\pi^2/3 + 40(\pi^2\log 2)/3 + 88\log^4 2 \\
&\quad +464\log^2 2 - 40\log 2
\end{aligned}
$$

where $\mathrm{Li}_n(x)$ is the polylog function. D_2, D_3 and D_4 were originally provided to us by mathematical physicist Craig Tracy, who hoped that our tools could help identify D_5.

The Ising Integral E_5

We were able to reduce E_5, which is a 5-D integral, to an extremely complicated 3-D integral.

We computed this integral to 250-digit precision, using a highly parallel, high-precision 3-D quadrature program. Then we used a PSLQ program to discover the evaluation given on the previous page.

We also computed D_5 to 500 digits, but were unable to identify it. The digits are available if anyone wishes to further explore this question.

$$
\begin{aligned}
E_5 \;=\; & \int_0^1 \int_0^1 \int_0^1 [2(1-x)^2(1-y)^2(1-xy)^2(1-z)^2(1-yz)^2(1-xyz)^2 \\
& (-[4(x+1)(xy+1)\log(2)(y^5z^3x^7 - y^4z^2(4(y+1)z+3)x^6 - y^3z((y^2+1)z^2+4(y+ \\
& 1)z+5)x^5 + y^2(4y(y+1)z^3+3(y^2+1)z^2+4(y+1)z-1)x^4 + y(z(z^2+4z \\
& +5)y^2+4(z^2+1)y+5z+4)x^3 + ((-3z^2-4z+1)y^2-4zy+1)x^2 - (y(5z+4) \\
& +4)x-1)] / [(x-1)^3(xy-1)^3(xyz-1)^3] + [3(y-1)^2y^4(z-1)^2z^2(yz \\
& -1)^2x^6 + 2y^3z(3(z-1)^2z^3y^5 + z^2(5z^3+3z^2+3z+5)y^4 + (z-1)^2z \\
& (5z^2+16z+5)y^3 + (3z^5+3z^4-22z^3-22z^2+3z+3)y^2 + 3(-2z^4+z^3+2 \\
& z^2+z-2)y + 3z^3+5z^2+5z+3)x^5 + y^2(7(z-1)^2z^4y^6 - 2z^3(z^3+15z^2 \\
& +15z+1)y^5 + 2z^2(-21z^4+6z^3+14z^2+6z-21)y^4 - 2z(z^5-6z^4-27z^3 \\
& -27z^2-6z+1)y^3 + (7z^6-30z^5+28z^4+54z^3+28z^2-30z+7)y^2 - 2(7z^5 \\
& +15z^4-6z^3-6z^2+15z+7)y + 7z^4-2z^3-42z^2-2z+7)x^4 - 2y(z^3(z^3 \\
& -9z^2-9z+1)y^6 + z^2(7z^4-14z^3-18z^2-14z+7)y^5 + z(7z^5+14z^4+3 \\
& z^3+3z^2+14z+7)y^4 + (z^6-14z^5+3z^4+84z^3+3z^2-14z+1)y^3 - 3(3z^5 \\
& +6z^4-z^3-z^2+6z+3)y^2 - (9z^4+14z^3-14z^2+14z+9)y + z^3+7z^2+7z \\
& +1)x^3 + (z^2(11z^4+6z^3-66z^2+6z+11)y^6 + 2z(5z^5+13z^4-2z^3-2z^2 \\
& +13z+5)y^5 + (11z^6+26z^5+44z^4-66z^3+44z^2+26z+11)y^4 + (6z^5-4 \\
& z^4-66z^3-66z^2-4z+6)y^3 - 2(33z^4+2z^3-22z^2+2z+33)y^2 + (6z^3+26 \\
& z^2+26z+6)y + 11z^2+10z+11)x^2 - 2(z^2(5z^3+3z^2+3z+5)y^5 + z(22z^4 \\
& +5z^3-22z^2+5z+22)y^4 + (5z^5+5z^4-26z^3-26z^2+5z+5)y^3 + (3z^4- \\
& 22z^3-26z^2-22z+3)y^2 + (3z^3+5z^2+5z+3)y + 5z^2+22z+5)x + 15z^2+2z \\
& +2y(z-1)^2(z+1) + 2y^3(z-1)^2z(z+1) + y^4z^2(15z^2+2z+15) + y^2(15z^4 \\
& -2z^3-90z^2-2z+15) + 15] / [(x-1)^2(y-1)^2(xy-1)^2(z-1)^2(yz-1)^2 \\
& (xyz-1)^2] - [4(x+1)(y+1)(yz+1)(-z^2y^4 + 4z(z+1)y^3 + (z^2+1)y^2 \\
& -4(z+1)y + 4x(y^2-1)(y^2z^2-1) + x^2(z^2y^4 - 4z(z+1)y^3 - (z^2+1)y^2 \\
& +4(z+1)y+1) - 1)\log(x+1)] / [(x-1)^3x(y-1)^3(yz-1)^3] - [4(y+1)(xy \\
& +1)(z+1)(x^2(z^2-4z-1)y^4 + 4x(x+1)(z^2-1)y^3 - (x^2+1)(z^2-4z-1) \\
& y^2 - 4(x+1)(z^2-1)y + z^2-4z-1)\log(xy+1)] / [x(y-1)^3y(xy-1)^3(z- \\
& 1)^3] - [4(z+1)(yz+1)(x^3y^5z^7 + x^2y^4(4x(y+1)+5)z^6 - xy^3((y^2+ \\
& 1)x^2 - 4(y+1)x - 3)z^5 - y^2(4y(y+1)x^3 + 5(y^2+1)x^2 + 4(y+1)x + 1)z^4 + \\
& y(y^2x^3 - 4y(y+1)x^2 - 3(y^2+1)x - 4(y+1))z^3 + (5x^2y^2 + y^2 + 4x(y+1) \\
& y+1)z^2 + ((3x+4)y+4)z - 1)\log(xyz+1)] / [xy(z-1)^3z(yz-1)^3(xyz-1)^3])] \\
& / [(x+1)^2(y+1)^2(xy+1)^2(z+1)^2(yz+1)^2(xyz+1)^2] \; dx\, dy\, dz
\end{aligned}
$$

2-D Integral in Bessel Moment Study

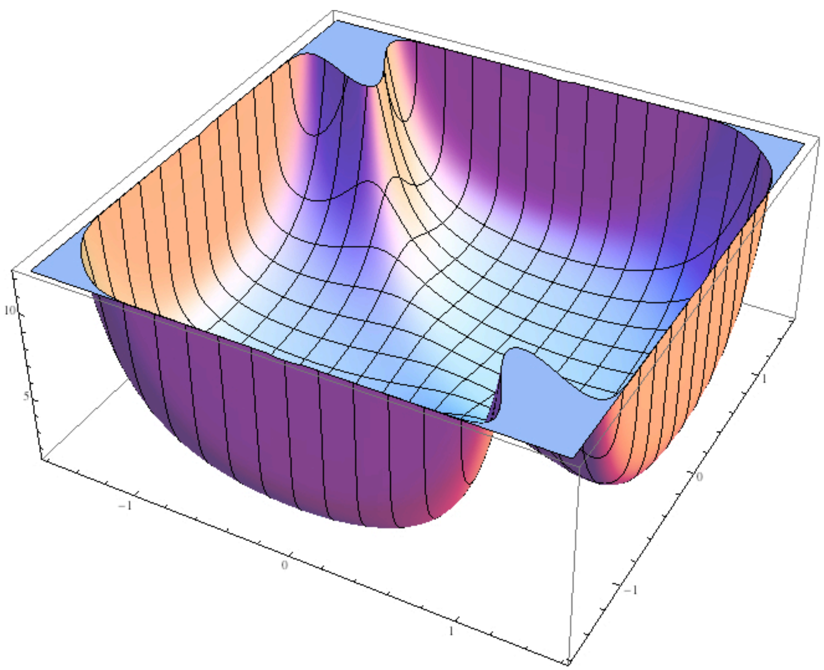
We conjectured (and later proved)

$$c_{5,0} \quad = \quad \frac{\pi}{2} \int_{-\pi/2}^{\pi/2} \int_{-\pi/2}^{\pi/2} \frac{\mathbf{K}(\sin\theta)\,\mathbf{K}(\sin\phi)}{\sqrt{\cos^2\theta\cos^2\phi + 4\sin^2(\theta+\phi)}}\,\mathrm{d}\theta\,\mathrm{d}\phi$$

Here **K** denotes the complete elliptic integral of the first kind

Note that the integrand function has singularities on all four sides of the region of integration.

We were able to evaluate this integral to 120-digit accuracy, using 1024 cores of the “Franklin” Cray XT4 system at LBNL.



DHB, J. M. Borwein, D. Broadhurst and M. L. Glasser, “Elliptic Integral Evaluations of Bessel Moments,” *Journal of Physics A: Math. and Gen.*, vol. 41 (2008), pg. 205203.

Box Integrals

The following integrals appear in studies, say, of the average distance between points in a cube, or the average electric potential in a cube:

$$B_n(s) \quad := \quad \int_0^1 \cdots \int_0^1 \left(r_1^2 + \cdots + r_n^2\right)^{s/2} \; dr_1 \cdots dr_n$$

$$\Delta_n(s) \quad := \quad \int_0^1 \cdots \int_0^1 \left((r_1 - q_1)^2 + \cdots + (r_n - q_n)^2\right)^{s/2} \; dr_1 \cdots dr_n \; dq_1 \cdots dq_n$$

DHB, J. M. Borwein and R. E. Crandall, "Box Integrals," *Journal of Computational and Applied Mathematics*, vol. 206 (2007), pg. 196-208.

Evaluations of Box Integrals

$$
\begin{aligned}
B_2(-1) &= \log\left(3+2\sqrt{2}\right) \\
B_3(-1) &= -\frac{\pi}{4} - \frac{1}{2}\log 2 + \log(5+3\sqrt{3}) \\
B_1(1) &= \frac{1}{2} \\
B_2(1) &= \frac{\sqrt{2}}{3} + \frac{1}{3}\log\left(\sqrt{2}+1\right) \\
B_3(1) &= \frac{\sqrt{3}}{4} + \frac{1}{2}\log\left(2+\sqrt{3}\right) - \frac{\pi}{24} \\
B_4(1) &= \frac{2}{5} + \frac{7}{20}\pi\sqrt{2} - \frac{1}{20}\pi\log\left(1+\sqrt{2}\right) + \log(3) - \frac{7}{5}\sqrt{2}\arctan\left(\sqrt{2}\right) + \frac{1}{10}\mathcal{K}_0
\end{aligned}
$$

where

$$
\mathcal{K}_0 := \int_0^1 \frac{\log(1+\sqrt{3+y^2}) - \log(-1+\sqrt{3+y^2})}{1+y^2}\,dy = 2\int_0^1 \frac{\operatorname{arctanh}\left(\frac{1}{\sqrt{3+y^2}}\right)}{1+y^2}\,dy
$$

Evaluations of Box Integrals, Cont.

$$
\begin{aligned}
\Delta_2(-1) &= \frac{4}{3} - \frac{4}{3}\sqrt{2} + 4\log(1+\sqrt{2}) \\
\Delta_1(1) &= \frac{1}{3} \\
\Delta_2(1) &= \frac{1}{15}\left(2+\sqrt{2}+5\log(1+\sqrt{2})\right), \\
\Delta_3(1) &= \frac{4}{105} + \frac{17}{105}\sqrt{2} - \frac{2}{35}\sqrt{3} + \frac{1}{5}\log(1+\sqrt{2}) + \frac{2}{5}\log(2+\sqrt{3}) - \frac{1}{15}\pi, \\
\Delta_4(1) &= \frac{26}{15}\,\mathrm{G} - \frac{34}{105}\,\pi\sqrt{2} - \frac{16}{315}\,\pi + \frac{197}{420}\,\log(3) + \frac{52}{105}\,\log\left(2+\sqrt{3}\right) \\
&+ \frac{1}{14}\,\log\left(1+\sqrt{2}\right) + \frac{8}{105}\,\sqrt{3} + \frac{73}{630}\,\sqrt{2} - \frac{23}{135} + \frac{136}{105}\,\sqrt{2}\arctan\left(\frac{1}{\sqrt{2}}\right) \\
&- \frac{1}{5}\,\pi\,\log\left(1+\sqrt{2}\right) + \frac{4}{5}\,\alpha\,\log\left(1+\sqrt{2}\right) - \frac{4}{5}\,\mathrm{Cl}_2\left(\alpha\right) - \frac{4}{5}\,\mathrm{Cl}_2\left(\alpha+\frac{\pi}{2}\right)
\end{aligned}
$$

where *G* is Catalan's constant and Cl denotes the Clausen function.

New Result (18 Jan 2009)

$$
\begin{aligned}
\Delta_3(-1) &= \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{(-1 + e^{-u^2} + \sqrt{\pi}\, u \operatorname{erf}(u))^3}{u^6} \, \mathrm{d}u \\
&= \frac{1}{15} \left(6 + 6\sqrt{2} - 12\sqrt{3} - 10\pi + 30 \log(1 + \sqrt{2}) + 30 \log(2 + \sqrt{3}) \right)
\end{aligned}
$$

As in many of the previous results, this was found by first computing the integral to high precision (250 to 1000 digits), conjecturing possible terms on the right-hand side, then applying PSLQ to look for a relation. We now have proven this result.

This and similar integrals have recently arisen in problems suggested by Stanford neuroscientists – e.g., the average distance between synapses in a mouse brain.

Ref: Work in progress! Will be written up soon.

High-Precision Arithmetic is Indispensible in Modern Scientific Computing

- State-of-the-art large-scale scientific calculations involving highly nonlinear systems often require numerical precision beyond conventional 64-bit floating-point arithmetic.
- Few physicists, chemists and engineers are experts in numerical analysis, so software-based high-precision arithmetic is often the best remedy for severe numerical round-off error.
- The emerging “experimental” methodology in mathematics and mathematical physics often requires hundreds or even thousands of digits of precision.
- Double-double, quad-double and arbitrary precision software libraries are now widely available (and in most cases are free).
- High-level C, C++ and Fortran-90 interfaces facilitate the conversion of large scientific programs to use this software.
- There is a critical need to develop much faster techniques for numerical integration in multiple dimensions.